3.1 Hydrogen Production

Hydrogen can be produced from a diversity of energy resources, using a variety of process technologies. Energy resource options include fossil, nuclear and renewables. Examples of process technologies include thermochemical, biological, electrolytic and photolytic.

Codes & Standards Safety Systems Integration/Analyses DELIVERY PRODUCTION FUEL CELLS TECHNOLOGY VALIDATION STORAGE Research & Development

3.1.1 Technical Goal and Objectives

Goal

Research and develop low-cost, highly efficient hydrogen production technologies from diverse, domestic sources, including natural gas and renewable sources.

Objectives

- By 2010, reduce the cost of distributed production of hydrogen from natural gas to \$1.50/gge² (delivered, untaxed) at the pump (without carbon sequestration).³
- By 2015, reduce the cost of distributed hydrogen production from biomass-derived renewable liquids to \$2.50/gge (delivered, untaxed) at the pump.
- By 2010, verify distributed grid-connected water electrolysis at a projected delivered hydrogen cost of \$2.85/gge. By 2015, verify renewable central hydrogen production at a projected cost of \$2.75/gge delivered.
- By 2015, reduce the cost of hydrogen produced from biomass to \$1.60/gge at the plant gate (\$2.60/gge delivered) by developing reforming technologies for gasification and pyrolysis processes.
- Develop advanced renewable photoelectrochemical and biological hydrogen generation technologies. By 2015, verify the feasibility of these technologies to be competitive in the long term.
- By 2015, develop high-temperature thermochemical cycles driven by concentrated solar power processes to produce hydrogen with a projected cost of \$3/gge at the plant gate (\$4.00/gge delivered).⁴
- Evaluate other new technologies that have the potential for cost-effective sustainable production of hydrogen and fund appropriate research and development in promising areas.

3.1.2 Technical Approach

Hydrogen production research is focused on meeting the objectives outlined in Section 3.1.1. by conducting R&D through industry, national laboratory, and university projects.

¹ Coal-based and nuclear-based hydrogen production are being addressed by the DOE Offices of Fossil Energy and Nuclear Energy, Science and Technology, respectively.

² The energy content of a gallon of gasoline and a kilogram of hydrogen are approximately equal on a lower heating value basis; a kilogram of hydrogen is approximately equal to a gallon of gasoline equivalent (gge) on an energy content basis.

³ \$1.50 is the estimated cost for hydrogen to be competitive for transportation systems in the 2015 timeframe. This estimate is currently under evaluation.

⁴ Collaboration with DOE's Office of Nuclear Energy, Science and Technology.

Technical Plan-Hydrogen Production

An array of feedstocks and technologies for hydrogen production will be necessary to address energy security and environmental needs. This program element addresses multiple feedstock and technology options for hydrogen production for the short and long terms. The research focus for the transition to a hydrogen infrastructure is on distributed reforming of natural gas and renewable liquid fuels, and on electrolysis to meet initial lower volume hydrogen needs with the least capital investment. The research focus is on renewable feedstocks and energy sources for the long term, with more emphasis on centralized options to take advantage of economies of scale when an adequate hydrogen delivery infrastructure is in place. There is a strong collaboration with DOE's Office of Fossil Energy to develop centralized production from coal with carbon sequestration, and with DOE's Office of Nuclear Energy, Science and Technology to develop centralized production from advanced nuclear energy-driven high-temperature thermochemical cycles and high temperature electrolysis. DOE's Office of Science is a collaborator on long-term technologies such as biological and photoelectrochemical hydrogen production.

The planned development of a national hydrogen production infrastructure will take multiple pathways. Some of these pathways and their roles within the strategy of the Hydrogen Production Program element are described below.

Distributed Production Pathway

Distributed production of hydrogen may be the most viable approach for introducing hydrogen as an energy carrier. It requires less capital investment for the smaller volume of hydrogen needed initially, and it does not require a substantial hydrogen transport and delivery infrastructure.

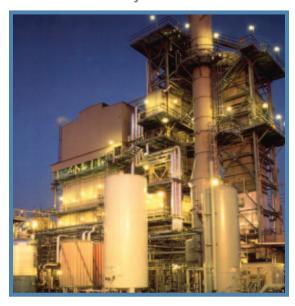
Two distributed hydrogen production technologies that have the best potential for development and commercialization during a transition to a hydrogen economy are 1) reforming of natural gas or liquid fuels, including renewable liquids such as ethanol and bio-oil, and 2) small-scale water electrolysis located at the point of use, i.e., refueling stations and stationary power generation sites. Of these technologies, natural gas reformers are in the most mature stage of development and are the closest to meeting the hydrogen production cost targets. Research will focus on developing these technologies through 2010, and then on applying them to reforming renewable liquid feedstocks for a competitive hydrogen cost. Distributed reforming using renewable liquids offers near-zero net greenhouse gas emissions. The second research focus is on small-scale electrolyzers

for splitting water. Electrolyzers present the opportunity for non-carbon-emitting hydrogen production when a renewable electricity source such as wind or hydro power is used. When off-peak electricity is used, greater economic opportunities may be presented by energy stations that produce both fuel and electricity.

Centralized Production Pathway

Large hydrogen production facilities that can take advantage of economies of scale will be needed in the long term to meet hydrogen fuel demand (see Figure 3.1.3). Central hydrogen production allows management of greenhouse gas emissions through strategies like carbon sequestration. In parallel with the distributed production effort, DOE is pursuing central production of hydrogen from a variety of resources-fossil, nuclear and renewable. Coal and natural gas are possibly the least expensive feedstocks, and carbon sequestration is required to reduce or eliminate greenhouse gas emissions. Reforming of

Figure 3.1.1 Centralized Hydrogen Production Facility



biomass gases or liquids offers a renewable option and near-zero greenhouse gas emissions. Centralized natural gas is not being pursued for the long-term because of energy security issues. Biomass reforming of gas or oils offers renewable feedstocks with near-zero net greenhouse gas emissions. Photoelectrochemical and biological hydrogen production are long-term technologies that have the potential to produce hydrogen with sunlight, but they can currently only produce small amounts of hydrogen at high cost. Centralized water electrolysis is a viable approach where there is inexpensive and low-carbon electricity. However, as the cost of capital equipment is reduced through advanced development, the cost of electricity becomes the dominant factor in the cost of hydrogen. High-temperature thermochemical hydrogen production that uses concentrated solar heat may be viable with the development of appropriate water-splitting chemical process cycles and materials. Other feedstocks and technologies for hydrogen production that show promise may also be considered.

Central production of hydrogen could potentially include a more diversified feedstock base, but to be commercially viable it would require development of a distribution infrastructure for hydrogen. The Program is pursuing projects to identify a cost-effective, energy-efficient, safe infrastructure for the delivery of hydrogen or hydrogen carriers from centrally located production facilities to the point of use (see section 3.2).

Other Production Pathways

Another pathway being explored is combined production of hydrogen, heat, and electric power. In this scenario, hydrogen would be produced for use in a higher temperature stationary fuel cell to produce electricity and heat as well as for use as a transportation fuel in fuel cell vehicles or hydrogen internal combustion engines. This allows two markets for the hydrogen in a swing plant operation, which could help to initiate the use of hydrogen when hydrogen demand is small. As the demand grows, more of the hydrogen could be produced for vehicle fuel rather than used for power production.

Much of the research is applicable to several of the production options. For example, advanced technology for reforming, shift, hydrogen separations, and hydrogen purification broadly applies to natural gas, coal, and biomass feedstocks and to both distributed and central production situations. Advanced hydrogen separation and purification technology is also common to many hydrogen production routes.

The Hydrogen Production Program element will develop the technologies to produce hydrogen for transportation and stationary applications. System validations will be performed by the Technology Validation Program element. Results of validation projects will guide continued R&D efforts.

3.1.3 Programmatic Status

Current Activities

Major Hydrogen Production Program element activities are listed in Table 3.1.1.

Challenge	Approach	Activities
Cost reduction of distributed hydrogen	Improve reforming and separation efficiencies	Praxair: Low-cost production platform using design for manufacture and assembly
production from natural gas and renewable liquids	Identify more durable reforming catalysts Incorporate breakthrough	Air Products and Chemicals Inc: Hydrogen refueling station using advanced natural gas steam methane reforming technologies
	separations technology	General Electric: Fuel-flexible autothermal cyclic reformer
	Reduce space needed Optimize system operation Intensify and consolidate the	National Renewable Energy Laboratory (NREL): Lower-cost technology for distributed reforming of biomass pyrolysis-derived bio-oils
number of steps, unit operations		Pacific Northwest National Laboratory (PNNL): Lower-cost technology to reform biomass-derived liquids such as sugars, sugar alcohols, and ethanol via liquid-phase or gasphase reforming
		Argonne National Laboratory (ANL): Novel technology to reform natural gas using high-temperature membranes and water splitting
		ANL: High-pressure ethanol reforming technology combined with more efficient separations and purification
		Virent Energy Systems, LLC, U. of Wisconsin, Archer Daniels Midland, UOP: Novel one-step liquid-phase reforming of carbohydrates
		H ₂ Gen Innovations, Süd-Chemie, Inc., Naval Research Lab: Advanced Steam Methane Reformer and Pressure Swing Adsorption Turn-Key Hydrogen Production System
		GE Global Research, University of Minnesota, Argonne National Laboratory: Integrated short-contact-time natural gas/bio- derived feedstock, compact reformer
		The BOC Group, Inc., Membrane Reactor Technologies Ltd., HERA USA Inc.: Integrated hydrogen production, purification and compression system
		Ohio State University Research Foundation: Ethanol steam reforming
Biomass-to-hydrogen	Develop advanced, lower- cost reforming technologies for hydrogen production from biomass gasification/pyrolysis	Gas Technology Institute, NETL, U. of Cincinnati, Allegheny Technology Company: Novel technology for one-step gasification, reforming, shift, and H ₂ separation
	,	United Technologies Research Center, U. of North Dakota: Innovative integrated slurry-based biomass hydrolysis and reforming process for low-cost hydrogen production

Biological production of hydrogen ^s	 Develop modifications to green algae, cyanobacteria, photosynthetic bacteria, and dark fermentative microorganisms that will facilitate efficient production of hydrogen Develop biochemical and process methods to facilitate efficient production of hydrogen Identify and develop costeffective components such as transparent, hydrogenimpermeable materials for photoreactors 	NREL, Oak Ridge National Laboratory (ORNL), UC Berkeley, IBEA, Montana State University, and Advanced Bionutrition: Identification of the physical and chemical variables needed to optimize biological systems based on new algal, cyanobacterial, photosynthetic bacterial, and dark fermentative microorganism strains; research the feasibility of various materials for photoreactors Benneman Associates: High-rate and yield hydrogen fermentation (SBIR)
Photoelectrochemical hydrogen production from water (direct water splitting) ⁵	 Develop high-efficiency materials Improve the durability of materials Develop photoelectrochemical devices and systems Identify and develop cost-effective components such as transparent, hydrogen-impermeable materials for photoreactors 	NREL, University of Hawaii, UC Santa Barbara, SRI, MV Systems, GE Global Research, and Midwest Optoelectronics: Identify and develop durable and efficient photoelectrochemical material(s), devices and systems
Hydrogen production from water via electrolysis	Reduce electricity costs of hydrogen production by developing new materials and systems to improve efficiency Reduce capital costs of electrolysis system through new designs with lower cost materials Develop low-cost hydrogen production from electrolysis using wind and other renewable electricity sources	Teledyne Energy Systems: New alkaline electrolysis materials for higher efficiencies and pressures Proton Energy Systems: Higher pressure PEM electrolysis system and renewable integration Giner Electrochemical Systems: PEM electrolysis system capable of electrochemical pressurization to 5000 psi with reduced capital costs; low-cost solid membranes (SBIR) Arizona State University: Combinatorial development of watersplitting catalysts for high efficiency electrolysis Ceramatec, Inc.: Large area cell for hybrid solid oxide hydrogen co-generation process General Electric: High-temperature reversible electrolysis materials and system development SRI International: Modular high-temperature system for hydrogen generation National Renewable Energy Laboratory: Research on renewable electrolysis power electronics integration Sandia National Laboratory: New high-efficiency, high-current-density alkaline membrane and electrode materials Avalence: High-efficiency ultra high-pressure electrolysis with direct linkage to photovoltaic arrays (SBIR) Ceramatec, Inc.: Novel bidirectional power controller for regenerative fuel cells.

⁵ In collaboration with DOE Office of Science.

High-temperature, solar-driven thermochemical cycles for splitting water to produce hydrogen ⁶	•Utilize the high-temperature energy from concentrated solar power to produce hydrogen through thermochemical cycles	Stirling Energy Systems, Inc., U. of Alabama, Weizmann Institute, CT LLC, U. of Massachusetts-Boston: Novel technology for solar-powered, low-voltage, high-efficiency production of hydrogen from water Science Applications International Corporation, Florida Solar Energy Center, U. of Turabo, U. of Central Florida: Evaluation of solar-driven carbon dioxide cycles for hydrogen production; pilot-scale testing of most promising system University of Colorado: Manganese-based solar-driven high-temperature thermochemical cycle to split water
Separation and purification systems (cross-cutting research) ⁷	Develop separation technology for distributed and central hydrogen production	Praxair: Integrated ceramic membrane system Sandia National Laboratories (SNL): Defect-free thin film membranes for hydrogen separation and purification Oak Ridge National Laboratory (ORNL): Inorganic membrane porous support tube fabrication and pyrochlore/perovskite ion transport membrane Media and Process Technologies, Johnson Matthey Catalyst, ChevronTexaco, University of Southern California: Carbon molecular sieve; membrane in a single-step shift reactor Pall Corporation, ChevronTexaco, Colorado School of Mines, Oak Ridge National Laboratory: Palladium alloy membrane U. of Cincinnati, Ohio State University, New Mexico Institute of Technology: Zeolite membrane reactor for single-step water gas shift reaction

3.1.4 Technical Challenges

The overarching technical challenge to hydrogen production is reducing cost. Hydrogen currently (as of 2003) costs \$5/gge delivered to a car at a refueling station (see Table 3.1.2) based on distributed production using natural gas, compared to the goal of \$1.50/gge (untaxed) in 2010. Estimates of the delivered cost of hydrogen using currently available technology for all production feedstocks is considerably higher than that required for hydrogen to be a cost-competitive primary energy carrier.

The capital costs of current electrolysis systems, along with the high cost of electricity in many regions, limit widespread adoption of electrolysis technology for hydrogen production. Electrolyzer capital cost reductions and efficiency improvements are required along with the design of utility-scale electrolyzers capable of grid integration and compatible with low-cost, near-zero emission electricity sources. Electrolytic production of hydrogen, where coal is the primary energy resource, will not lead to carbon reduction without carbon sequestration technologies.

Hydrogen can be produced from biomass either by distributed reforming of bio-derived liquids or through gasification or pyrolysis of biomass feedstocks. The costs of currently-available bio-derived liquids such as ethanol or sugar alcohols (e.g. sorbitol) need to be reduced. Significant improvements in ethanol reforming and new technologies need to be developed for other bio-derived liquids to reduce the capital and operating costs

⁶ In collaboration with DOE Office of Nuclear Energy, Science and Technology.

⁷ In collaboration with DOE Office of Fossil Energy.

for this production option to become competitive. The efficiencies of biomass gasification or pyrolysis and reforming need to be increased and the capital costs need to be reduced by developing improved technologies and approaches.

Biological hydrogen production is in an early stage of research and presents many technical challenges, beginning with molecular engineering of microorganisms that can produce hydrogen at high rates. However, the advantages of biological hydrogen production are that high-purity water is not required and toxic or polluting byproducts are not generated.

Photoelectrochemical hydrogen production (direct water splitting), also in an early stage of development, depends on a breakthrough in materials development and could require large areas of land. Research in this area is progressing on three fronts: 1) the study of high-efficiency materials in order to attain the basic science understanding needed for improving lower-efficiency lower-cost materials; 2) the study of low-cost durable materials in order to attain the basic science understanding needed for modifying higher-efficiency lower-durability materials; and 3) the development of multijunction devices incorporating multiple material layers to achieve efficient water splitting.

High-temperature, solar-driven, thermochemical hydrogen production using water-splitting chemical cycles is in an early stage of research. Research is also needed to cost-effectively couple the thermochemical cycles with advanced concentrated solar power technology. If these efforts are successful, high-temperature thermochemical processes may provide a clean, efficient, and sustainable route for producing hydrogen from water.

3.1.4.1 Technical Targets

A variety of feedstocks and processes are being researched and developed for producing hydrogen fuel. Each technology is in a different stage of development, and each offers unique opportunities, benefits, and challenges. Economics favor certain technologies more than others in the near term, but other technologies are expected to become economically viable as the technologies mature and market conditions shift.

Tables 3.1.1 through 3.1.12 list the DOE technical targets for hydrogen production from a variety of feedstocks. All targets were developed through preliminary hydrogen production analyses and will be refined further as the technology matures and trade-offs are identified. The targets and timeline for each technology reflect a number of factors, including the expected size of a production unit, the stage of technology development, and the costs and characteristics of the feedstock.

Targets for 2010 and 2015 are R&D milestones for measuring progress and are not necessarily the targets required for successful commercialization of the technology. For hydrogen to become a major energy carrier, the combination of its cost and that of the power system it is used in, must be competitive with the alternatives available in the market. For personal transportation light duty vehicles, this means that the combination of the hydrogen cost, and its use in a hydrogen fuel cell vehicle, must be competitive with gasoline internal combustion engine powered vehicles, or other alternatives, on a cost/mile basis to the consumer. The estimated cost of hydrogen needed to be competitive with gasoline is \$1.50/gge delivered (untaxed) at the dispenser. This estimate is currently being re-evaluated to reflect projected fuel costs and vehicle power system energy efficiencies on a cost per mile basis. The ultimate target for all of the production technologies being researched is a hydrogen cost that will be competitive for transportation on a well-to-wheels basis, regardless of the production pathway.

All targets must be achieved simultaneously; however, status is not neccessarily reported from a single system.

Fixed O&M Cost Contribution

Feedstock Cost Contribution

Other Variable O&M Cost Contribution

Table 219	Technical Target	e: Dictributed Dradi	uction of Hydrogen	from Natural Gas a, b
LIANIC J. I.Z.	Tecillical faluer	3. DISHIDULGU FIVU	UGUUN ON MYUNUGN	II UIII Naturai yas 🔧

		Calendar Year			
Characteristics	Units	2003° Status	2005 ^d Target	2010 ^d Target	
Total Energy Efficiency ^e	%(LHV)	65.0	65.0	75.0	
Production Energy Efficiency	%(LHV)	69.0	69.0	80.0	
Storage, Compression, and Dispensing Energy Efficiency ^f	%(LHV)	94.0	94.0	94.0	
Total Hydrogen Cost	\$/gge H ₂	5.00	3.00	1.50	
Detailed Cost Breakdown – These calculations are for guidance only and not necessarily the research targets to achieve the total energy efficiency and cost goals.					
Capital Cost Contribution	\$/gge H ₂	2.70	1.40	0.30	
Production	\$/gge H ₂	1.90	0.60	0.10	
Storage, Compression, Dispensing ^f	\$/gge H ₂	0.80	0.80	0.20	

\$/gge H₂

\$/gge H₂

\$/gge H₂

1.20

0.90

0.20

0.60

0.80

0.20

0.30

0.70

0.20

^a Economic parameters used were for a production design capacity of 1500 kg/day of hydrogen: 20 yr. analysis period, 10% IRR after taxes, 100% equity financing, 1.9% inflation, 38.9% total tax rate, and MACRS 7-year depreciation. A 70% capacity factor was used for 2003 and 2005. A 90% capacity factor was used for 2010. The results in 2000\$\$ were inflated by 6% to yield 2003\$\$.

b The natural gas price was set to \$4.50/MMBTU in 2000\$, based on the levelized price for natural gas between 2005 and 2025 based on the EIA AEO 2004 for industrial rates. The electricity price was set at \$.07/kWhr in 2000\$ based on the levelized price between 2005-2025 based on the EIA AEO 2004 for commercial rates.

[°] For the 2003 analysis it was assumed the units would be built a few at a time.

^d For the 2005 and 2010 analysis it was assumed that Design for Manufacture and Assembly (DFMA) would be employed and that on the order of 500 units per year would be produced.

^e Energy efficiency is defined as the energy of the hydrogen out of the process (LHV) divided by the sum of the energy into the process from the feedstock (LHV) and all other energy needed. The electrical energy utilized does not include the efficiency losses from the production of the electricity.

Storage capacity for 1100 kg of hydrogen at the forecourt is included. It is assumed that the required hydrogen pressure for refueling is 5000 psi for 2003 and 2005. It is assumed that in 2015, the pressure for hydrogen refueling is 1500 psi.

Table 3.1.3. Technical Targets: Distributed Production of Hydrogen from Bio-Derived Renewable Liquids ^{a,b}

Kenewabie Liquids ***						
		Calendar Year				
Characteristics	Units	2003° Status	2005° Target	2010° Target	2015 ^d Target	
Total Energy Efficiency ^e	%	46.0	46.0	66.0	70.0	
Production Energy Efficiency	%	49.0	49.0	70.0		
Storage, Compression, Dispensing Energy Efficiency ^f	%	94.0	94.0	94.0		
Total Hydrogen Cost	\$/gge	6.70	5.90	3.60	2.50	
Detailed Cost Breakdown – These calculations are for guida the total energy efficiency and cost goals.	nce only and	not necessa	rily the resea	rch targets to	o achieve	
Capital Cost Contribution	\$/gge	1.90	1.30	0.90		
Production	\$/gge	1.10	0.50	0.50		
Storage, Compression, Dispensing ^f	\$/gge	0.80	0.80	0.40		
Fixed O&M Cost Contribution	\$/gge	0.70	0.50	0.40		
Feedstock Cost Contribution ^g	\$/gge	3.80	3.80	1.80		
Other Variable O&M Cost Contribution	\$/gge	0.30	0.30	0.50		

^a Economic parameters used were 20 yr. analysis period, 10% IRR after taxes, 100% equity financing, 1.9% inflation, 38.9% total tax rate, MACRS 7-year depreciation, 70% capacity factor. 2000\$ calculations were inflated by 6% to yield 2003\$.

b The electricity price was set at \$.07/kWhr in 2000\$ based on the levelized price between 2005-2025 based on the EIA AEO 2004 for commercial rates.

c The 2003 status, 2005, and 2010 target are based on an initial analysis of distributed reforming of ethanol at a design capacity of 1500 kg/day of hydrogen based on available information.

d The 2015 target is based on what might be achievable with breakthroughs in technology and alternative bio-derived renewable liquids.

^e Energy efficiency is defined as the energy of the hydrogen out of the process (LHV) divided by the sum of the energy into the process from the feedstock (LHV) and all other energy needed. The electrical energy utilized does not include the efficiency losses from the production of the electricity

f Storage capacity for 1100 kg of hydrogen at the forecourt is included. It is assumed that the required hydrogen pressure for refueling is 5000 psi for 2003 and 2005. It is assumed that in 2015, the pressure for hydrogen refueling is 1500 psi.

For 2003 and 2005 the price of ethanol used is \$1.15/gallon in 2003\$. This is a typical price for ethanol in the fuel market over the past 5 years. For 2010, the price of ethanol used is \$.85/gallon in 2003\$. It is assumed that this cost reduction is possible based on using less purified and wet ethanol (i.e. only using a single distillation step rather than two distillation steps and molecular sieve drying currently used in ethanol manufacture from corn), further improvements in ethanol production from corn and/or the introduction of other lower cost ethanol production technology such as from cellulosic biomass.

Table 3.1.4. Technical Targets: Water Electrolysis ^a							
1500 kg/day refueling station			Central Renewable ^b				
Characteristics		Units	2003 Status	2005 Target	2010 Target	2015 Target	
Power Conversion, Cell Stack, Balance of Plant ^c	Cost	\$/gge H ₂	0.95	0.80	0.39	0.24	
	Total Cell Efficiency	%	66	68	76	77	
	Cost	\$/gge H ₂	0.83	0.77	0.19	0.08	
Compression, Storage, Dispensing	Efficiency	%	94	94	99	99.5	
Electricitye	Cost	\$/gge H ₂	2.57	2.47	1.89	1.32	
O&M	Cost	\$/gge H ₂	0.80	0.71	0.38	0.11	
	Cost	\$/gge H ₂	5.15	4.75	2.85	2.75 ^g	
Total ^f	Efficiency	%	62	64	75	76	

^a Economic parameters used were: 20 yr. analysis period, 10% IRR after taxes, 100% equity financing, 1.9% inflation, 38.9% total tax rate, MACRS 7-year depreciation, 70% capacity factor. The H2A results in 2000\$ were inflated by 6% to yield 2003\$.

Hydrogen separation is a key component that cross-cuts most, if not all of the hydrogen production technology options. The separation membranes described in Tables 3.1.5 and 3.1.6 have multiple applications requiring an array of system configurations. Separations systems that best reduce the cost to produce hydrogen more efficiently from diverse feedstocks will be downselected. These separations sub-system components must be optimized to achieve the cost and hydrogen quality requirements. Tables 3.1.5 and 3.1.6 present targets for three major hydrogen separation technology pathways and reflect the current stage of development for each as well as the need to achieve performance requirements within the timeframe of the 2015 commercialization decision. The performance requirements presented are based on a preliminary set of assumptions with regard to system configuration (feedstock composition, temperature, pressure, and product composition). Ultimately, though, success will be determined based on analysis of the actual system configuration and its requirements.

b Renewable Option: Calculation base on delivering 50,000 gge hydrogen per day (1000+ gge modules) with option of electricity co-production. Electricity back up provided by grid.

^c Includes power conversion, cell stack and balance of plant (efficiency based on AC electric input to hydrogen output on a LHV basis).

d Compression improvements result from integral electrochemical or other system compression to reduce or eliminate mechanical compression. Lower pressure storage assumed in 2015.

^e Electricity at EIA projected industrial electricity rate for 2003-2005. \$.04 per kWh assumed in 2010 based on regional industrial electricity rate and new renewable technologies on the grid. \$.03 per kWh assumed in 2015 with central wind and grid back up. \$.03 per kWh also corresponds to the Office of Wind and Hydropower 2012 production cost goal for class 4 wind resources.

f Based on system capital cost per kWe of \$700, \$600 and \$250 for the refueling station in 2003, 2005 and 2010, respectively, and \$200 for the central station in 2015. Assumes high volume annual production (1,000 units for all purposes and all markets) of electrolyzer units in 2010-2015 and centralized facility benefiting from scale on installation.

Includes \$1.00 per gge delivery charge (transportation to the station, hauling and dispensing).

Table 3.1.5. Technical Targets: Dense Metallic Membranes for Hydrogen Separation and Purification

. allioation						
		Calendar Year				
Performance Criteria ^a	Units	2003 Status	2005 Target	2010 Target	2015 Target	
Flux Rate ^c	scfh/ft²	60	100	200	300	
Membrane Material and All Module Costs ^d	\$/ft² of membrane	2,000	1,500	1,000	<500	
Durabilitye	hr	<8,760 ^f	8,760	26,280	>43,800	
ΔP Operating Capability ^g	psi	100	200	400	400-1,000	
Hydrogen Recovery	% of total gas	60	>70	>80	>90	
Hydrogen Quality ^h	% of total (dry) gas	>99.9	>99.9	>99.95	99.99	

^a The membranes must be tolerant to impurities. This will be application specific. Common impurities include sulfur and carbon monoxide.

Notes: Revised targets take into consideration input received at the September, 2004 H₂ Separations Workshop. These targets are undergoing detailed engineering analysis. Membrane systems should be demonstrated within a temperature range between 250-1,000 degrees Celsius. Also, parasitic power requirements (that used to recompress the hydrogen downstream of the membrane due to potential pressure drops across the membrane) should be minimized.

^b Based on membrane shift reactor with syngas.

^c Flux at 20 psi hydrogen partial pressure differential with a minimum permeate side total pressure of 15 psi, preferably >50 psi and 400 °C.

^d The membrane support structure is approximately three times membrane material costs.

^e Intervals between membrane replacement.

^f Hydrogen membranes have not been demonstrated to date, only laboratory tested.

^g Delta P operating capability is application dependent. There are many applications that may only require 400 psi or less. For coal gasification 1000 psi is the target.

h Based on current available PEM fuel cell information, the tentative contaminant targets are: <10ppb sulfur, <1 ppm carbon monoxide, <100 ppm carbon dioxide, <1 ppm ammonia, <100 ppm non-methane hydrocarbons on a C-1 basis, oxygen, nitrogen and argon can not exceed 2% in total, particulate levels must meet ISO standard 14787.

Table 3.1.6	Technical Targets: Microporous Membranes for Hydrogen Separation and
	Purification

Performance Criteria ^a	Units	2003 Status	2005 Target	2010 Target	2015 Target
Flux Rate ^b	scfh/ft²	100	100	200	300
Membrane Material and All Module Costs ^c	\$/ft² of Membrane	450-600	400	200	<100
Durability ^d	hr	<8,760°	8,760	26,280	>43,800
ΔP Operating Capability ^f	psi	100	200	400	400-1000
Hydrogen Recovery	% of total gas	60	>70	>80	>90
Hydrogen Quality ^g	% of total (dry) gas	≥90	95	99.5	99.99

Note: Revised targets take into consideration input received at the September, 2004 H, Separations Workshop. These targets are undergoing detailed engineering analysis. Membrane systems should be demonstrated within a temperature range between 250-1,000 Degrees Celsius. Also, parasitic power requirements (that used to recompress the hydrogen downstream of the membrane due to potential pressure drops across the membrane) should be minimized.

The membranes must be tolerant to impurities. This will be application specific. Common impurities include sulfur and carbon monoxide. Flux at 20 psi hydrogen partial pressure differential with a minimum permeate side total pressure of 15 psi, preferably >50 psi and 400 $^{\circ}$ C.

The membrane support structure cost is approximately three times more than membrane material costs.

Intervals between membrane replacement.

Hydrogen membranes have not been demonstrated to date, only laboratory tested.

Delta P operating capability is application dependent. There are many applications that may only require 400 psi or less. For coal gasification 1000 psi is the target.

Based on current available PEM fuel cell information, the tentative contaminant targets are: <10ppb sulfur, <1 ppm carbon monoxide, <100 ppm carbon dioxide, < 1 ppm ammonia, < 100 ppm non-methane hydrocarbons on a C-1 basis, oxygen, nitrogen and argon can not exceed 2% in total, particulate levels must meet ISO standard 14787.

Table 3.1.7. Technical Targets: Biomass Gasification/Pyrolysis Hydrogen Production ^a						
		Calendar Year				
Characteristics	Units	2003 Status	2005 Target	2010 Target	2015 Target	
Energy Efficiency ^b	%	44	47	50	52	
Total Hydrogen Cost	\$/gge H ₂	2.10	1.90	1.75	1.60	
Detailed Cost Breakdown – These calculations at the total energy efficiency and cost goals.	are for guidance	e only and not r	necessarily the	research target	s to achieve	
Capital Cost Contribution	\$/gge H ₂	0.70	0.60	0.55	0.50	
Feedstock Cost Contribution ^c	\$/gge H ₂	0.70	0.65	0.60	0.50	
Fixed O&M Cost Contribution	\$/gge H ₂	0.40	0.40	0.35	0.35	
Other Variable O&M Cost Contribution	\$/gge H ₂	0.30	0.25	0.25	0.25	

^a Economic parameters used were: 40 yr. analysis period, 10% IRR after taxes, 100% equity financing, 1.9% inflation, 38.9% total tax rate, MACRS 20-year depreciation. The results in 2000\$ were inflated by 6% to yield 2003 dollars. These costs are at the plant gate. The cost target for delivery of hydrogen from the plant gate to the point of refueling at a refueling station in 2015 is \$1.00/gge (See Section 3.2).

b Energy efficiency is defined as the energy of the hydrogen out of the process (LHV) divided by the sum of the energy into the process from the feedstock (LHV) and all other energy needed. The electrical energy utilized does not include the efficiency losses from the production of the electricity.

^c For 2003 and 2005 a biomass feedstock cost of \$46/dry ton in 2000\$ was used. For 2010 a feedstock cost of \$44/dry ton was used. For 2015 a feedstock cost of \$42/dry ton was used.

Table 3.1.8. Technical Targets: Photolytic Biological Hydrogen Production from Water ^a						
Characteristics	Units	2003 Status	2010 Target ^b	2015 Target ^{c,d}		
Utilization Efficiency of Incident Solar Light Energy (E0*E1)e	%	10	15	20		
Efficiency of Incident Light Energy to Hydrogen from Water (E0*E1*E2) ^f	%	0.1	2	5		
Duration of Continuous Photoproduction ^g	Time Units	not available ^g	30 min	4 hr		
O ₂ Tolerance (half life in air)	Time Units	1 sec	10 min	2 hr		

	E0		E1		E2
Solar Light		Absorbed Light		Electrons	→ H ₂

^a Hydrogen cost will be evaluated as part of the research and development Go/No-Go decision in 2015 (see Appendix B). The targets in this table are for research tracking. The final targets for this technology are to reach costs that are competitive with traditional fuels for transportation applications and with other hydrogen production technologies.

^b 2010 target is based on analysis of best technologies available, theoretically integrated into a single organism.

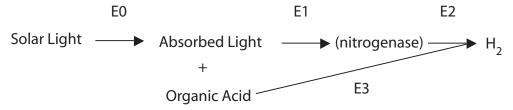
c 2015 targets are based on analysis of best technologies available, actually integrated into a single organism.

d Near commercialization targets (beyond 2015) are 25% utilization efficiency of incident solar light energy (E0*E1), 10% efficiency of incident light energy to H, from water (E0*E1*E2), ≥12h (O₂ tolerant) duration of continuous photoproduction, and 6h O₂-tolerance (half-life in air).

^e E0 reflects the light collection efficiency of the photoreactor and the fact that only a fraction of solar incident light is photosynthetically active (theoretical maximum is 45%). E1 is the efficiency with which algae convert the energy of absorbed photons to chemical energy (i.e. chemical potential; theoretical maximum is 71%). E0*E1 represents the efficiency of conversion of incident solar light to chemical potential (theoretical maximum is 32%). E2 reflects the efficiency with which the chemical potential generated by the absorbed photons is converted to hydrogen (theoretical maximum is 41%). E0*E1*E2 represents the efficiency of conversion of incident solar light to H₂ (theoretical maximum is 13% when water is the substrate); only peak efficiencies are meant.

g Duration reflects continuous production in the light, not necessarily at peak efficiencies. Targets reflect oxygen tolerant system.

Table 3.1.9. Technical Targets: Photosynthetic Bacterial Hydrogen Production ^a					
Characteristics	Units	2003 Status	2010 Target	2015 ^b Target	
Efficiency of Incident Solar Light Energy to H ₂ (E0*E1*E2)° from organic acids	%	1.9 ^d	3	4.5	
Molar Yield of Carbon Conversion to H ₂ (depends on nature of organic substrate) E3 ^e	% of maximum	42 ^e	50	65	
Duration of continuous photoproduction ^f	Time	6 days ^g	30 days	3 months	



- ^a Hydrogen cost will be evaluated as part of the research and development Go/No-Go decision in 2015 (see Appendix B). The targets in this table are for research tracking. The final targets for this technology are to reach costs that are competitive with traditional fuels for transportation applications and with other hydrogen production technologies.
- b Near commercialization targets (beyond 2015) are 5.5% efficiency of incident solar light energy to H₂ (E0*E1*E2) from organic acids, 80% of maximum molar yield of carbon conversion to H₂ (depends on nature of organic substrate) E3, and 6 months duration of continuous photoproduction.
- ^c E0 reflects the light collection efficiency of the photoreactor and the fact that only a fraction of incident solar light is photosynthetically active (theoretical maximum is 68%, from 400 to 1000 nm). E1*E2 is equivalent to the efficiency of conversion of absorbed light to primary charge separation then to ATP; both are required for hydrogen production via the nitrogenase enzyme. E0*E1*E2 represents the efficiency of conversion of incident solar light to hydrogen through the nitrogenase enzyme (theoretical maximum is 10% for 4-5 electrons). This efficiency does not take into account the energy used to generate the carbon substrate.
- ^d Average from data presented by Akkerman, I., M. Janssen, J. Rocha, and R. H. Wijffels. 2002. Intl. J. Hydrogen Energy 27: 1195-1208.
- ^e E3 represents the molar yield of H₂ per carbon substrate (the theoretical maximum is 7 moles per mol carbon in the substrate, in the case of acetate and butyrate). Average of data presented by Koku, H., I. Eroglu, U. Gunduz, M. Yucel, and L. Turker. 2002. Intl. J. Hydrogen Energy 27: 1315-1329.
- f Duration reflects continuous production in the light, not necessarily at peak efficiencies. It includes short periods during which ammonia is re-added to maintain the system active.
- g Average from data presented by Koku, H., I. Eroglu, U. Gunduz, M. Yucel, and L. Turker. 2002. Intl. J. Hydrogen Energy 27: 1315-1329.

Table 3.1.10. Technical Targets: Dark Fermentative Hydrogen Production ^a					
Characteristics	Units	2003 Status	2010 Target	2015 Target ^b	
Yield of H ₂ production from glucose ^c	mol H ₂ mol glucose	2 ^d	4	6	
Feedstock Coste	cents/lb sugar	13.5	10	8	
Duration of continuous production	Time	17days ^f	3 months	6 months	

- ^a Hydrogen cost will be evaluated as part of the research and development Go/No-Go decision in 2015 (see Appendix B). The targets in this table are for research tracking. The final targets for this technology are to reach costs that are competitive with traditional fuels for transportation applications and with other hydrogen production technologies.
- ^b Near commercialization targets (beyond 2015) are 10 molar yield of H₂ Production from glucose, 6 cents/lb sugar feedstock cost, and 12 months duration of continuous production.
- ^c The theoretical maximum from known fermentative pathways is 4, although the H₂ content of 1 mole of glucose is 12. Clearly, in order to achieve molar yields greater than 4, the feasibility of developing new pathways or discovering new microbes needs to be assessed.
- ^d DOE Workshop on Hydrogen Production via Direct Fermentation (June 2004) and Boundary Analysis for H₂ Production by Fermentation, publications in preparation
- ^e Targets set by the DOE Biomass Program for glucose from lignocellulosic biomass. NREL Report TP-510-32438 http://www.nrel.gov/docs/fy02osti/32438.pdf; NREL E Milestone #586, May 2004.
- ^f Van Ginkel, S., and S. Sung. 2001. Environ. Sci. Technol.,35: 4726-4730.

Table 3.1.11. Technical Targets: Photoelectrochemical Hydrogen Production ^a						
Characteristics	Units	2003 Status	2010 Target	2015 Target [®]		
Usable semiconductor bandgap ^c	eV	2.8	2.3	2.0		
Chemical conversion process efficiency (EC) ^d	%	4	10	12		
Plant solar-to-hydrogen efficiency (STH) ^e	%	not available	8	10		
Plant durability ^f	hr	not available	1000	5000		

^a Hydrogen cost will be evaluated as part of the research and development Go/No-Go decision in 2015 (see Appendix B). The targets in this table are for research tracking. The final targets for this technology are to reach costs that are competitive with traditional fuels for transportation applications and with other hydrogen production technologies.

f Durability reflects projected duration of continuous photoproduction, not necessarily at peak efficiencies.

Table 3.1.12. Solar-Driven High-Temperature Thermochemical Hydrogen Production ^a					
Characteristics	Units	2005 Target	2010 Target	2015 Target	
Solar-Driven High-Temperature Thermochemical Cycle Hydrogen Cost	\$/gge H ₂	10	6	3	
Solar Concentrator Capital Cost (installed cost) ^b	\$/m²	200	170	130	
Process Energy Efficiency ^c	%	30	40	45	

^a Based on initial analysis. Two potential high temperature cycles were examined: the Westinghouse modified sulfur cycle with electrolysis, and a zinc oxide cycle. The capacity basis was central production of 150,000 kg/day of hydrogen. All targets are expressed in 2003 dollars. These costs are at the plant gate. The cost target for delivery of hydrogen from the plant gate to the point of refueling at a refueling station in 2015 is \$1.00/gge (See Section 3.2)

b Near commercialization targets (beyond 2015) are 16% plant solar-to-hydrogen efficiency (STH) and 15,000 hours plant durability.

^c The bandgap of the interface semiconductor establishes the photon absorption limits. Useable bandgaps correspond to systems with adequate stability, photon absorption and charge collection characteristics for meeting efficiency, durability and cost targets.

d EC reflects the process efficiency with which a semiconductor system can convert the energy of absorbed photons to chemical energy [based on AM (Air Mass) 1.5 insolation] and is a function of the bandgap, IPEC and electronic transport properties. A multiple junction device may be used to reach these targets.

^e Solar-to-hydrogen (STH) is the projected plant-gate solar-to-hydrogen conversion efficiency based on AM (Air Mass) 1.5 insolation. Both EC and STH represent peak efficiencies, with the assumption that the material systems are adequately stable.

b These capital cost targets are consistent with those of the EERE Solar Program for a heliostat field and tower. They do not include the receiver.

^c The process energy efficiency is defined as the energy of the hydrogen produced (LHV) divided by the sum of the energy from the solar concentrator plus any other net energy required for the process. The solar concentrator energy efficiency targets are the same as for the EERE Solar Program.

3.1.4.2 Barriers

The following sections detail the technical and economic barriers that must be overcome to attain the Hydrogen Production goal and objectives. The barriers are divided into sections depending on the hydrogen production method.

3.1.4.2.1 Distributed Hydrogen Production from Natural Gas or Renewable Liquid Feedstocks

- A. Fuel Processor Capital Costs. Current small-scale distributed natural gas and renewable liquid feedstock reforming technologies have capital costs that are too high to achieve the targeted hydrogen production cost. Multiple unit operations and low energy efficiencies are key contributors to the high capital costs. Improved reforming and shift catalysts are needed to reduce side reactions and improve performance. Shift, separation, and purification costs need to be reduced. Process intensification by combining steps could significantly reduce costs. For example, combining the current two step shift and PSA separation into a one-step shift with integrated hydrogen separation could significantly reduce capital costs.
- **B.** Fuel Processor Manufacturing. Distributed reforming units are currently designed and built one at a time, particularly for large industrial applications. Efforts such as Design for Manufacture and Assembly (DFMA) need to be applied to develop more compact, appliance-type units that can be produced using low-cost, high-throughput manufacturing methods.
- C. Operation and Maintenance (O&M). O&M costs for distributed reforming hydrogen production from natural gas and renewable feedstocks are too high. Robust systems that require little maintenance and that include remote monitoring capability need to be developed.
- **D**. **Feedstock Issues**. Availability of some feedstocks is limited in certain areas. Feedstock-flexible reformers are needed to address location-specific feedstock supply issues. Effects of impurities on the system from multiple feedstocks as well as the effects of impurities from variations in single feedstocks need to be addressed in the reformer design.
- E. Carbon Dioxide Emissions. Distributed natural gas reformers emit greenhouse gases. Cost-effectively sequestering these relatively smaller volume and highly distributed carbon emissions is significantly more challenging than at central hydrogen production facilities that use fossil fuels. Feedstocks and/or technologies that can approach near zero net greenhouse gas emissions are needed.
- **F.** Control and Safety. Control and safety issues are associated with natural gas and renewable feedstock reforming, including on-off cycling. Effective operations control strategies are needed to minimize cost and emissions, maximize efficiencies, and enhance safety. Hydrogen leakage is addressed within the Delivery and Safety Program elements.

3.1.4.2.2 Hydrogen Generation by Water Electrolysis

G. Capital Cost. The capital costs of electrolysis systems are prohibitive to widespread adoption of electrolysis technology for hydrogen production. R&D is needed to develop lower cost materials with improved manufacturing capability to lower capital while improving the efficiency and durability of the system. Development of larger systems is also needed to improve economies of scale.

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- H. System Efficiency. New membrane, electrode and system designs are needed to improve system efficiency. Mechanical high-pressure compression technology exhibits low energy efficiency and often reduces hydrogen purity while adding significantly to the system cost. Efficiency gains can be realized using electrochemical compression in the cell stack. Low-cost, high-pressure materials need to be developed to provide integral electrochemical or other high-pressure compression technologies to replace some or all mechanical compression stages. Development is needed for low-cost cell stack optimization considering efficiency, electrochemical compression, and durability.
- **I. Grid Electricity Emissions**. The current grid electricity mix in most locations increases greenhouse gas emissions in large-scale electrolysis systems. Low-cost, carbon-free electricity sources are needed.
- J. Renewable Integration. More efficient integration with renewable electricity sources is needed to reduce costs and improve performance. Development of integrated renewable electrolysis systems is needed, including optimization of power conversion and other system components from renewable electricity to provide high-efficiency, low-cost integrated renewable hydrogen production. Novel concepts for carbon-free electrolytic hydrogen production need to be evaluated.
- **K.** Electricity Costs. High-temperature solid oxide electrolysis can use lower cost energy in the form of steam for water splitting to decrease electricity consumption. Technically viable systems for low-cost manufacturing need to be developed for this technology. Electrolysis systems that can produce both hydrogen and electricity need to be evaluated. (Renewable electricity costs will be addressed by the DOE EERE renewable power programs Solar, Wind, Hydropower, Geothermal and Biomass.)

3.1.4.2.3 Separations and Other Cross-Cutting Hydrogen Production

There are a number of technology options available that can be used to separate and purify hydrogen. The following is a set of broad, cross-cutting barriers that must be overcome to reduce the cost and increase the efficiency of these separation technologies.

- L. Durability. Since hydrogen is noncorrosive, special materials of construction are not usually required; however, hydrogen embrittlement occurs in some metals. Hydrogen can embrittle certain types of membranes used in separation technologies, inducing a phase change. Embrittlement reduces the durability and effectiveness of the membrane for selectively separating hydrogen. Thermal cycling can cause failure in some membranes, reducing their durability and operating life. This is especially problematic in distributed applications that are subject to frequent start-up and shut-down cycles. Finally, materials do not perform optimally. Support structures with more uniform pore sizes and less surface roughness are needed to avoid membrane defects. Interactions between membrane and support structure materials need to be better understood. Fundamental materials science work is needed to understand microstructural evolution during operation and effect on membrane permeance, selectivity, and failure modes. Combinatorial methods are needed for rapid testing and evaluation of novel materials and alloys.
- **M.** Impurities. The presence of trace contaminants as well as CO, water, and CO₂ in the exit gas from a gasifier or reformer can reduce the hydrogen flux across different types of membranes. It is not understood whether these effects are caused by competitive adsorption or compositional changes on the membrane surface. Additionally, some membranes exhibit poor thermochemical stability in carbon dioxide environments, resulting in the conversion of membrane materials into carbonates. In solvent systems, impurities can cause less effective absorption and may lead to excessive loss of solvent, which will increase cost. Non-reversible adsorption of impurities onto the surface of metallic membranes can poison the

membrane and lead to total failure. Researchers and membrane developers need a better understanding of the concentrations of all trace components in the feed gas stream so that membrane systems can be designed and tested for tolerance to these contaminants. PEM fuel cells require a highly pure hydrogen product containing: CO < 1 ppm, $CO_2 < 100$ ppm, S < 10 ppb, $NH_3 < 1$ ppm, non-methane hydrocarbons < 100 ppm and O_2 , N_2 , Ar < 2%.

- N. Defects. Oxidizing gas mixtures (oxygen, steam, and carbon oxides) have been observed to cause metallic membranes to rearrange their atomic structure at temperatures greater than 450 °C. This results in the formation of defects that reduce membrane selectivity for hydrogen. High-temperature and high-pressure seals are difficult to make using ceramic substrates. Seals and joints are a weak link in membrane module construction and one of the most common points of membrane system failure. Large-scale (high-yield, low-cost) manufacturing methods for defect-free thin films and membranes and modules in mass production must be developed and demonstrated. Fabrication of defect-free membranes requires a reduction in membrane deposition cycles. The chemical deposition of thin palladium or palladium-alloy membranes onto support structures is also an important technical challenge. Vapor deposition and solution plating offer the ability to rapidly produce very thin films, but current technologies are defect prone and susceptible to contamination.
- **O. Selectivity.** The hydrogen selectivity of microporous membranes is lower than desired for cost-effective use, especially for zeolite-supported membranes where selectivity decreases with increasing temperature (inadequate above 150 °C). However, temperatures typically need to be greater than 300 °C in various applications.
- **P. Operating Temperature.** Processes that can be designed to operate at or near system conditions, without the need for cooling and/or re-heating, will be more efficient. For example, dense ceramic proton hydrogen separation membranes currently operate only at high temperatures (~900 °C). Separation systems suitable for distributed reforming of natural gas and renewable liquids are needed. Low temperature systems (< 50 °C) are needed for biological and photoelectrochemical systems.
- **Q.** Flux. Flux rates for membranes need to be improved to reduce the membrane size and lower overall cost of hydrogen separation and purification systems.
- **R.** Testing and Analysis. Better information is needed to guide researchers and membrane technology developers towards performance targets that are application specific. Standard methods for evaluating and screening membrane materials and modules are needed to provide a solid basis for comparison of alternatives and to conduct needed tests such as accelerated durability tests. Testing under real-world operating conditions is needed to demonstrate durability and robust, reliable performance. Additionally, there is currently a lack of understanding of tradeoffs between different system configurations and operating parameters. Operation at higher temperatures and partial pressure differentials can increase flux rates but results in more expensive membrane modules. Very thin membranes increase flux but they are harder to fabricate defect-free. Analysis is also needed to understand options and tradeoffs for process intensification in different applications.
- **S. Cost.** In addition to precious metals, membrane materials and support structures are costly. Even metallic membranes, where small amounts of precious metals are used, are more costly than non-metallic membranes.

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- **T.** Oxygen Separation Technology. Commercial oxygen separation technology relies on expensive and energy-intensive cryogenic separation. Low-cost oxygen membrane technology needs to be developed for potential use in distributed reforming, biomass gasification/pyrolysis and other hydrogen production technologies.
- U. High-Purity Water Availability. Impacts on water supplies are not understood. Further analysis is needed.

3.1.4.2.4 Biomass Gasification/Pyrolysis Hydrogen Production

- V. Feedstock Cost and Availability. Feedstock costs are high. Improved feedstock/agriculture technology (higher yields per acre, etc.), lower cost feedstock collection, and improved feedstock preparation are needed. Because biomass feedstocks are often seasonal in nature, feedstock-flexible processes and/or cost-effective feedstock storage are needed (Tasks to overcome these barriers will be developed by the DOE Biomass Program and the U.S. Department of Agriculture).
- W. Capital Cost and Efficiency of Biomass Gasification/Pyrolysis Technology. The capital cost for biomass gasification/pyrolysis needs to be reduced. Process intensification by combining steps can significantly reduce capital costs. This could range from combining the current two step shift and PSA separation to a one step shift with integrated separation, to integrating gasification, reforming, shift and separation all in one unit. Improved process efficiency and higher hydrogen yields and selectivities through catalyst research, better heat integration, and alternative gas clean-up approaches are needed. Improved catalysts or engineering approaches for tar cracking are also needed.

3.1.4.2.5 Biological Hydrogen Production

A number of technologies for biological H₂ production are available, but they are not mature at present. Technical barriers related to each individual technology must be overcome, integrated models must be developed, and barriers related to an integrated system must be identified before economic barriers can be meaningfully considered. Methods for engineering and manufacturing these systems have not been fully evaluated. Barriers are listed below for each technology, followed by a model for how these different technologies could be integrated and a list of barriers for the integrated process.

Photolytic H₂ Production from Water (green algae or cyanobacteria):

- X. Light Utilization Efficiency. The microorganisms used for photobiological H₂ production possess large arrays of light-capturing antenna pigment molecules. Under bright sunlight, pigment antennae absorb much more light than can be utilized by the photosynthetic electron transport apparatus, resulting in heat dissipation and loss of up to 80% of the absorbed sunlight. Research is needed to identify ways to increase the light conversion efficiency, including the identification of better and/or modified photosynthetic organisms for H₂ production.
- Y. Rate of Hydrogen Production. The current H₂ production rate from photosynthetic microorganisms is too low for commercial viability. The low rates have been attributed to (a) the non-dissipation of a proton gradient across the photosynthetic membrane, which is established during electron transport from water to the hydrogenase (the H₂-producing enzyme) under anaerobic conditions, and (b) the existence of competing metabolic flux pathways for reductant. Genetic means to overcome the restricting metabolic pathways, such as the insertion of a proton channel across the thylakoid membrane, must be used to significantly increase the rate of H₂ production. Under aerobic conditions, with an O₂-tolerant hydrogenase catalyzing H₂ production, the competition between CO₂ fixation and hydrogenase will have to be addressed.

- Z. Continuity of Photoproduction. Hydrogen-producing algae co-produce oxygen, which inhibits the hydrogenase enzyme activity. This inhibition needs to be alleviated, possibly by (a) identifying or engineering a less O₂-sensitive enzyme; (b) separating the oxygen and hydrogen production cycles; or (c) affecting the ratio of photosynthesis to respiration (P/R) by a variety of means, such that O₂ does not accumulate in the medium, the quantum yield of photosynthesis is maintained, and full hydrogenase activity is achieved (see details under Integrated System).
- AA. Systems Engineering. System requirements for cost-effective implementation of photolytic hydrogen-production technologies have not been adequately evaluated. Analysis and research are needed on inexpensive/transparent materials for H₂ containment, H₂ collection systems, prevention of the build-up of H₂/O₂ gas mixtures, separation of co-produced H₂ and O₂ gases, continuous bioreactor operation, monoculture maintenance, land area requirements and capital costs.
- **AB. Diurnal Operation Limitations.** Photolytic processes are discontinuous because they depend on sunlight, which is unavailable at night and available only at low intensities on cloudy days. This results in increased capital costs for larger facilities to accommodate higher short-term production rates and larger hydrogen storage needs. Engineering options need to be carefully analyzed to minimize capital requirements.

Photosynthetic Bacterial Hydrogen Production, Required for an Integrated System:

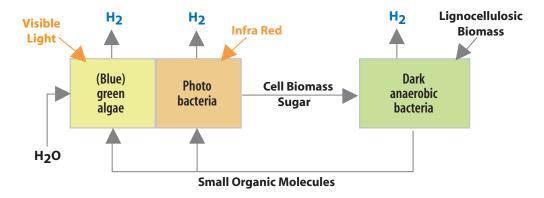
- AC. Light Utilization Efficiency. Same issues apply as for photolytic systems (see Barrier X).
- **AD. Rate of Hydrogen Production.** Photosynthetic bacteria can metabolize a variety of organic substrates that are waste by-products of various fermentative processes. However, the metabolism of acetic and lactic acids to H₂ also generates by-products such as polymer polyhydroxyalkanoate (PHA). Synthesis of PHA competes with H₂ production for the same source of electron donors. Genes controlling PHA synthesis and perhaps other pathways must be inactivated to maximize H₂ production. Alternative types of nitrogenase are needed to produce larger stoichiometric amounts of H₂/ammonia.
- **AE. Hydrogen Re-oxidation.** Most photosynthetic bacteria contain an H₂-oxidation pathway catalyzed by an uptake hydrogenase enzyme. This enzyme will recycle the H₂ produced by the nitrogenase to support cell growth. Uptake hydrogenase enzyme(s) must be inactivated to ensure net H₂ accumulation by photosynthetic bacteria.
- **AF.** Carbon/Nitrogen Ratio. To maximize nitrogenase activity, the proper ratio of carbon to nitrogen (C/N) nutrients must be maintained. The C/N nutrient content in the photoreactor (algal and cyanobacteria) and in the dark fermentor needs to be evaluated to assess whether the media composition is suitable for subsequent photosynthetic bacterial hydrogen production. Enzyme engineering approaches may be needed to alleviate inhibition of nitrogenase by elevated levels of nitrogen nutrient.
- **AG. Systems Engineering.** The same issues apply as for photolytic systems (see above), except for the mixture of gases. Photosynthetic bacteria do not co-evolve H₂ and O₂ but release H₂ and CO₂. The cost of H₂ and CO₂ separation must be evaluated.
- **AH. Diurnal Operation Limitation.** The same issues apply as for photolytic systems (see Barrier AB).

Dark Fermentative Hydrogen Production, Required for an Integrated System:

- **AI. H**₂ **Molar Yield.** Up to 4 moles of H₂ can theoretically be produced per mole of glucose through the known fermentative pathways. However, various biological limitations such as H₂-end-product inhibition and waste-acid and solvent accumulation limit the molar yield to around 2 moles per mole glucose consumed. Hydrogen molar yields must be increased significantly through metabolic engineering efforts. New pathways must be discovered to directly take full advantage of the 12 moles of H₂ available in a mole of glucose.
- **AJ. Waste Acid Accumulation.** Organic acids such as acetic and butyric acids are waste by-products of the fermentation process. The production of these acids poses several challenges such as lowering the molar yield of H₂ by diverting the metabolic pathway toward solvent production and requiring subsequent wastewater treatment. Elimination of this pathway or subsequent processing (such as in an integrated biological hydrogen production system) of the organic acids by photosynthetic bacteria is needed to increase hydrogen yields. Potential release of toxins during dark fermentation and their inhibition of the subsequent steps (such as in an integrated system) will need to be evaluated.
- **AK. Feedstock Cost.** The glucose feedstock is the major cost driver for economic H₂ production via fermentation. For renewable H₂ to be cost competitive with traditional transportation fuels, the glucose cost must be around \$0.05 per pound and provide a molar yield of H₂ approaching 10 (see Barrier AI and Target Table 3.1.9). Lower-cost methods for producing glucose from whole biomass are needed. Cellulolytic microbes with a high rate of H₂ production are also needed to use the cell biomass of the green algal/cyanobacterial and photosythetic bacterial co-culture (in an integrated biological H₂ production system).
- **AL. Systems Engineering.** The same issues apply as above, plus prevention of methanogen contamination is needed.

Integrated Biological Hydrogen Production System (many configurations are possible, Figure 3.1.2):

Figure 3.1.2. Integrated Biological System



Illustrative Scenario: Anaerobically, co-culture (blue) green algae and photosynthetic bacteria in a photoreactor, and dark anaerobic bacteria in a fermentor. Feedstock for the dark anaerobic bacteria is derived from the cell biomass/sugars of the (blue) green algae and the photosynthetic bacteria. Additional feedstock for the dark anaerobic bacteria is derived from lignocellulosic products. The small organic molecule by-products of the dark anaerobic bacterial fermentation are subsequently utilized as feedstock for the (blue) green algae and photosynthetic bacteria.

- AM. Photosynthesis/Respiration Capacity Ratio: Green algae and cyanobacteria become anaerobic when their P/R (photosynthesis/respiration) capacity ratio is 1 or less. Under such anaerobic conditions, photosynthetic water oxidation produces H_2 (instead of starch), and the O_2 evolved by photosynthesis is consumed by respiration, producing CO_2 . Currently, this process is achieved by nutrient deprivation, with the drawback that the resulting $P/R \le 1$ ratio is achieved by partially decreasing the quantum yield of photosynthesis. Alternative mechanisms to bring the P/R ratio to 1 need to be investigated, particularly those methods that focus on achieving a P/R ratio of 1 without changing the quantum yield of photosynthesis. Two further issues will need to be investigated under these conditions: (a) rate limitations due to the non-dissipation of the proton gradient and (b) the ability of the culture to take up a variety of exogenous carbon sources under the resulting anaerobic conditions.
- AN. Co-Culture Balance: To extend the absorption spectrum of the H₂-photoproducing cultures to the infrared (700-900 nm), the possibility of co-cultivating oxygenic photosynthetic organisms with anoxygenic photosynthetic bacteria should be investigated. However, in addition to light in the infrared region, photosynthetic bacteria also absorb light in the visible (400 to 600 nm), thus potentially competing with green algae for these latter wavelengths. Strategies need to be devised to either maintain the appropriate biomass ratio of the two organisms as suspensions in the same reactor, or to physically separate them in the same photoreactor via immobilization of one or both cultures. The competition for organic carbon substrates between two organisms in the same medium also needs to be investigated.
- AO. Concentration/Processing of Cell Biomass. In an integrated system, cell biomass from either green algae/cyanobacteria or photosynthetic bacteria can serve as the substrate for dark fermentation. The green algal and cyanobacterial cell walls are made mostly of glycoproteins, which are rich in arabinose, mannose, galactose and glucose. Purple photosynthetic bacterial cell walls contain peptidoglycans (carbohydrate polymers cross-linked by protein, and other polymers made of carbohydrate protein and lipid). Pretreatment of cell biomass may be necessary to render it more suitable for dark fermentation. Methods for cell concentration and processing will depend on the type of organism used and how the biological system is integrated.

3.1.4.2.6 Photoelectrochemical Hydrogen Production

Photoelectrochemical hydrogen production, in an early stage of development, depends on a breakthrough in materials development. The primary research in this area is progressing on three fronts: 1) the study of high-efficiency materials to attain the basic science understanding needed for improving lower-efficiency, low-cost materials; 2) the study of low-cost durable materials to attain the basic science understanding needed for modifying higher-efficiency, lower-durability materials; and 3) the development of multijunction devices incorporating multiple material layers to achieve efficient water splitting. Methods of engineering and manufacturing these systems need to be developed in conjunction with the materials and device research.

Current material systems for photoelectrochemical hydrogen production can broadly be divided into three categories, each with its own characteristics and research challenges. These groupings are: (i) stable materials with low visible light absorption efficiency (e.g. oxides), (ii) highly efficient light absorbers with low lifetimes (e.g. III-Vs) and (iii) hybrid and multijunction systems which combine multiple materials in multi-photon devices. The group (i) materials are characterized by high bandgaps and low integrated incident-photon-to-electron conversion (IPEC) over the solar spectrum; the group (ii) materials have very high IPEC (better than 90% throughout the visible spectra), but have low corrosion resistance and poor energetics; and the group (iii) systems can have very high efficiency and long lifetime, depending on the material set, but can be complicated and expensive to build. Research in all three categories is necessary for developing systems that meet the targets

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reflected in the PEC target table. To date, a range of materials and material systems have met individual 2010 targets of chemical efficiency or durability, but no single material/system has simultaneously met efficiency, durability and cost targets. This is the primary research challenge for photoelectrochemical hydrogen production.

- **AP. Materials Efficiency.** Materials with smaller bandgaps more efficiently utilize the solar spectrum, but are often less energetically favorable for hydrogen production because of the bandedge mismatch with respect to either hydrogen or oxygen redox potentials. Materials with appropriate bandedge and bandgap for hydrogen production must be developed.
- **AQ. Materials Durability**. Durable materials with the appropriate characteristics for photoelectrochemical hydrogen production that meet the Hydrogen Production Program element goals have not been identified. The high-efficiency materials currently available corrode quickly during operation, and the most durable materials are very inefficient for hydrogen production.
- **AR. Bulk Materials Synthesis.** Fabrication techniques for materials identified to have potential for high efficiency, durability and low cost need to be developed on scales consistent with implementation in commercial reactors.
- **AS. Device Configuration Designs**. Hybrid and other device designs that combine multiple layers of materials could address issues of durability and efficiency. Techniques are needed for manufacturing appropriate photoelectrochemical materials in these device configurations at commercial scales.
- AT. Systems Design and Evaluation. System designs incorporating the most promising device configurations, and using cost-effective, hydrogen-impermeable, transparent materials are also needed to implement photolytic production routes. The complete systems evaluation will need to consider a range of important operational constraints and parameters, including the diurnal operation limitations and the effects of water purity on performance and lifetime. Engineering options need to be carefully analyzed to minimize capital requirements.

3.1.4.2.7 High-Temperature Thermochemical, Solar-Driven Production of Hydrogen⁶

- **AU. High-Temperature Thermochemical Technology**. There are over 150 possible thermochemical cycles for solar driven water splitting. These cycles need to be evaluated and ranked for their suitability. The most promising cycles need to be more fully explored and verified to down select to a few cycles for research and development. Many of these cycles require the development of technology to either very rapidly quench high temperature reactions and/or separate hydrogen or other materials at high temperatures.
- **AV. High-Temperature Robust Materials**. High temperatures are employed in these thermochemical systems. Cost-effective, durable materials are needed that can withstand these high temperatures and the thermal duty cycles present in solar concentrator systems.
- **AW.** Concentrated Solar Energy Capital Cost. Concentrated solar energy collection is currently expensive and requires large areas of land. Improved, lower-cost solar concentrator/collection technology, including materials, is needed.⁷

⁶ DOE's Office of Nuclear Energy, Science and Technology has the lead responsibility for hydrogen production utilizing nuclear energy for high temperature (700°-1000°C) thermochemical water splitting chemical cycles. The Office of Hydrogen, Fuel Cells & Infrastructure Technologies will collaborate with Nuclear Energy, Science and Technology on the thermochemical hydrogen production R&D activities.

⁷ The Hydrogen Program will rely on and collaborate with the DOE EERE Solar Program for the advancement of concentrated solar energy technology.

AX. Coupling Concentrated Solar Energy and Thermochemical Cycles. Coupling concentrated solar energy with thermochemical cycles presents many challenges. Receivers and reactors need to be developed and engineered. Cost effective approaches and systems to deal effectively with the diurnal nature of sunlight need to be researched and developed.

3.1.5 Technical Task Descriptions

The technical task descriptions are presented in Table 3.1.10. Concerns regarding safety and environmental effects will be addressed within each task in coordination with the appropriate Program element.

Task	Description	Barriers
1	 Low-Cost, Distributed Production of Hydrogen from Natural Gas Develop advanced, small-scale reformer technology for greater efficiency, selectivity, and durability. Develop advanced shift catalysts that are more efficient and impurity tolerant. Evaluate pathways for improving conventional water-gas-shift catalysts and reactors, including single-stage shift. Develop advanced technology that integrates process steps and energy to minimize capital, unit size, and energy use in an intensified process. Utilize Design for Manufacture and Assembly (DFMA) to design appliance type units for high-thoughput low-cost manufacture. Design for robust operations that minimize maintenance and process monitoring needs. 	A, B, C, D E, F
2	Distributed Reforming of Renewable Liquid Feedstocks Analyze and research options for alternative renewable feedstocks (e.g., ethanol, methanol, sugar alcohols, bio-oils, bio-based Fischer Tropsch liquids) for distributed production. Utilizing the technology concepts developed for distributed natural gas reforming, develop efficient, integrated, compact, robust process technology for bio-derived liquid feedstocks. Explore novel technology for reforming bio-derived renewable liquid feedstocks that could result in a cost breakthrough.	A, B, C, D E, F
3	 Advanced Electrolysis Technologies to Reduce Cost and Increase Efficiency Reduce cell stack cost by developing lower cost durable materials with improved manufacturing capability optimized for efficiency, durability, and stack compression. Develop electrochemical and other novel compression technologies, integral to cell stacks, to reach hydrogen output pressures greater than 500 psi using low-cost materials. Optimize electrolysis with renewable energy systems to lower cost of power conversion and other system components. Develop utility-scale electrolysis system suitable for renewable and grid electricity integration. Develop system components for lower system O&M costs including cell stack durability and compression. Evaluate steam electrolysis for reducing electricity costs associated with hydrogen production and improving system durability. Continue development of reversible solid oxide electrolyzer materials and system design. 	G, H, I, J, K, U

4	 Separation and Purification Systems (Cross-Cutting Research) Develop a membrane reactor system that combines water-gas-shift reaction for hydrogen production with a membrane for hydrogen separation and purification in a single step to achieve reductions in system operations and maintenance costs as well as reductions in overall system capital costs. Investigate new lower-cost alloys to achieve fundamental improvements in metallic membrane technology to achieve necessary hydrogen purity levels. Overcome embrittlement and fracture issues associated with producing high-purity hydrogen at high concentrations to promote system durability. Verify that inorganic, metallic, and ion transport membrane systems can meet or exceed separation targets under realistic commercial operating conditions. Develop membranes that optimize hydrogen and carbon dioxide selectivity. Improve existing air separation technologies and identify novel technologies for separating oxygen for gasification and reforming. Develop integrated membrane/reactor systems for reforming. 	A, B, C, E, L, M, N, O, P, Q, R, S, T, V, W, AA, AG, AL, AS, AU, AV
5	Cost Reduction of Biomass Reforming for Gasification/Pyrolysis Identify all opportunities for reducing the cost of biomass gasification/pyrolysis technologies. Reduce the cost and increase the feedstock flexibility of biomass feedstock preparation (e.g. handling, size reduction, etc.) Research and develop more cost-effective, efficient, and durable biomass product gas clean up technologies for feed into reforming operations, including hot-gas clean-up, tar cracking, and other related technologies. (This will be coordinated with the Office of Fossil Energy for coal-gasifier product gas clean up technologies and with the EERE Biomass Program.) Investigate opportunities for catalyst and reactor improvement for reforming and conditioning of biomass producer gases. Improve process overall heat integration and improve hydrogen yields and selectivities to improve energy efficiency and reduce cost. Intensify and reduce the capital cost by combining/integrating process steps and operations. This could include single step shift with an integrated membrane, combining shift and reforming in one operation, combining gasification and reforming in one operation, etc. Develop other gasification/pyrolysis improvements, including further heat integration, reactor configurations, etc.	V, W
6	 Molecular and Physiological Engineering of Organisms for Photolytic Hydrogen Production from Water Generate organisms that are O₂-tolerant, have increased light conversion efficiency, allow more efficient photosynthetic electron transport toward H₂, and eliminate competing pathways for enhanced H₂ production. Eliminate H₂ uptake pathways in cyanobacteria. Research and develop systems in which water photolysis occurs under anaerobic conditions (i.e., in which the P/R ratio is ≤1). Test different methods to achieve that ratio without affecting H₂ production (priority for the development of an integrated system). Incorporate elements from the first bullet, if necessary. 	X,Y, Z
7	 Systems Engineering for Photolytic Hydrogen Production from Water Optimize photoreactor material and system designs. Discover and develop cost effective, transparent, H₂-impermeable materials for photolytic production of H₂. Develop hydrogen collection and gas separation technologies. Verify economic and technical viability of continuous hydrogen production. 	AA, AB

8	 Molecular Engineering of Organisms for Photosynthetic Bacterial Hydrogen Production Increase the useful portion of the solar spectrum beyond the visible and into the infrared by co-cultivating green algae/cyanobacteria and photosynthetic bacterial (priority for the development of an integrated system). Generate photosynthetic bacteria that have increased sunlight conversion efficiency and display more efficient photosynthetic electron transport. Eliminate competitive pathways such as H₂ oxidation and polymer accumulation. Engineer organisms that have a functional nitrogenase at elevated nitrogen-nutrient concentration. Investigate the H₂-production activity and solar efficiency of organisms containing alternative nitrogenases. 	AC, AD, AE, AF
9	 Systems Engineering for Photosynthetic Bacterial Hydrogen Production Optimize photoreactor material and system designs. Discover and develop cost effective, transparent, H₂-impermeable materials for photosynthetic bacterial H₂ production. Develop H₂-collection and gas-separation technologies. Verify economic and technical viability of continuous H₂ production. 	AG, AH
10	 Molecular Engineering of Organisms for Dark Fermentative Hydrogen Production Eliminate competing pathways for H₂ production. Bioprospect for cellulolytic microbes that can ferment cellulose along with mixed sugars, and for organisms with pathways that allow for higher H₂ molar yield. Investigate fermentation of green alga/photosynthetic bacteria cell biomass from the co-culture for H₂ production. Investigate the potential production of toxins by different fermentative organisms that could prevent integration with other components of the overall system. 	AI, AJ, AK
11	 Systems Engineering for Dark Fermentative Hydrogen Production Develop catalytic degradation processes of cell biomass to be more suitable for the subsequent dark fermentation. Industrial-scale enzymes, or chemical processes, need to be defined that can be applied in large scale for the catalytic breakdown of these cell wall biopolymers to their monomeric constituents. Dark anaerobic fermentations for the production of H₂ can then utilize the resulting sugars as a suitable feedstock. Develop H₂-collection and gas-separation technologies. Develop methanogen management approaches. 	AL
12	 Integrated Biological Hydrogen Production (dependent on configuration used) (see Figure 3.1.2) Investigate the best way to integrate anaerobic water photolysis (green algal and/or cyanobacterial H₂ production) with photosynthetic bacterial H₂ production. This could involve co-cultivation of organisms or immobilized cultures. Determine the efficacy of green algae/cyanobacteria and photosynthetic bacteria to metabolize different exogenous organic carbon substrates. Regulate competition (for sunlight and/or nutrients) between different organisms in the case of co-cultivation, and eliminate transfer of potential cell-growth inhibitors from the fermentor to the photoreactors. Investigate low-cost methods to concentrate/process organisms in suspension, as necessary. 	AM, AN, AO

13	 Development of Semiconductor Materials for Photoelectrochemical Hydrogen Production Develop and optimize the current state of the art materials for meeting near term efficiency and durability targets. Discover, utilizing combinatorial or other screening methods, new materials for meeting long-term efficiency, durability, and cost targets. Develop cost-effective synthesis techniques for fabricating the most promising semiconductor materials. Develop accelerated screening protocols to evaluate and validate long-term material efficiencies and durability. 	AP, AQ, AR
14	Material Configurations and Device Engineering for Photoelectrochemical Hydrogen Production Evaluate device configurations, including multi-junction configurations and other advanced designs, for improved efficiency and durability and lower device cost. Develop and optimize the most promising device configurations. Develop cost-effective fabricating synthesis techniques that are scalable and manufactureable for the most promising materials systems, devices, and configurations.	AP, AQ, AR, AS
15	Systems Development for Photoelectrochemical Hydrogen Production Design reactor systems to optimize light-capture efficiency, hydrogen production, gas collection and reactor life – including utilization of novel geometries and electrolyte options. Identify or develop auxiliary materials and components necessary for photoelectrochemical hydrogen production systems, including cost effective transparent, hydrogen-impermeable materials for reactors. Develop accelerated testing protocols to evaluate and validate long-term system efficiencies and durability. Apply economic modeling tools for predicting cost potentials for photolytic production technologies.	АТ
16	 High-Temperature, Solar-Driven, Thermochemical Processes Evaluate potential high-temperature, solar driven thermochemical water-splitting cycles and down-select to the most promising cycles. Develop a cost effective integration of concentrated solar power with high-temperature thermochemical water splitting cycles. Develop a viable integrated, solar-driven high-temperature thermochemical water-splitting process. Develop cost-effective, high-temperature materials compatible with thermochemical processes. Verify an integrated, solar-driven high-temperature thermochemical water-splitting cycle with targeted costs. 	AU, AV, AW, AX

3.1.6 Milestones

Figure 3.1.3 shows the interrelationship of milestones, tasks, supporting inputs from other Program elements, and technology outputs for the Hydrogen Production Program element from FY 2004 through FY 2012. This information is also summarized in Table B.1 in Appendix B.

FY 2003 FY 2004 FY 2005 FY 2006 FY 2007 FY 2008 FY 2010 FY 2011 FY 2012 Distributed Reforming Task 1: Low Cost, Distributed Production of Hydrogen from Natural Gas Task 2: Distributed Reforming of Renewable Liquid Feedstocks ⊟ectrolysis Task 3: Advanced Electrolysis Technologies to Reduce Cost and Increase Efficiency Separation and Purification (Cross-Cutting) Task 4: Separation and Purification Systems (Cross-cutting Research) Biomass Reforming Task 5: Cost Reduction of Biomass Reforming for Pyrolysis/Gasification **Photolytic Water Oxidation** Task 6: Molecular and Physiological Engineering of Organisms for Photolytic Hydrogen Production from Water Task 7: Systems Engineering for Photolytic Hydrogen Production from Water Photosynthetic Bacterial Hydrogen Production Task 8: Molecular Engineering of Organisms for Photosynthetic Bacterial Hydrogen Production Task 9: Systems Engineering for Photosynthetic Bacterial Hydrogen Production Milestone Input Output Go/No-go

Figure 3.1.3. Hydrogen Production R&D Milestone Chart

For chart details see next page.

Milestones

- 1 Down-select research for distributed natural gas-to-hydrogen production.
- 2 Select advanced shift catalysts that are more efficient and impurity tolerant.
- Werify feasibility of achieving \$1.50/gge (delivered) from distributed natural gas.
- 4 Verify feasibility of achieving \$3.60/gge for renewable liquids distributed reforming.
- 5 Down-select research for distributed production from bio-derived renewable liquids.
- 6 Go/No-Go: Decision on continued high-temperature steam electrolysis R&D based on a complete technoeconomic analysis and laboratory-scale research results.
- 7 Verify feasibility of achieving \$2.85/gge (delivered) from electrolysis.
- 8 Go/No-Go: Determine if membrane separation technology can be applied to natural gas distributed reforming during the transition to a hydrogen economy.
- 9 Down-select separation technology for development in distributed natural gas reforming.
- 10 Demonstrate pilot-scale use of integrated separation (membrane) reactor system for natural gas.
- 11 Down-select separation technology for distributed bio-derived renewable liquid feedstocks reforming.
- 12 Demonstrate pilot-scale use of integrated separation (membrane) reactor system for renewable feedstocks.
- 13 Down-select to a primary technology and configuration for biomass gasification/pyrolysis clean-up, reforming, shift, separation and purification.
- Verify a projected cost for biomass gasification/pyrolysis of \$1.75/gge at plant gate.
- Down-select to 1-2 primary novel technologies for biomass gasification/pyrolysis clean up, reforming, shift, separation and purification.
- 16 Identify or generate an Fe-hydrogenase with a half-life of 5 min in air for photolytic hydrogen production.
- 17 Produce one cyanobacterial recombinant evolving H, through an O,-tolerant NiFe-hydrogenase.
- 18 Increase the duration of H, production by immobilized, sulfur-deprived algal cultures to 40 days.
- 19 Complete research to develop a photosynthetically efficient green alga/cyanobacterial system in which the P/R ratio is ≤2.
- 20 For photolytic hydrogen production, achieve 15% primary utilization efficiency of incident solar light energy (E0*E1), 2% efficiency of incident light energy to H, from water (E0*E1*E2), and 30 min (O, tolerant system) duration of continuous photoproduction.
- 21 Identify or generate an Fe-hydrogenase with a half life of 30 min in air for photolytic hydrogen production.
- 22 Go/No-Go: Identify cost-effective (based on analysis) transparent H, -impermeable material for use in photobiological H, -production system.
- 23 Complete research to generate photosynthetic bacteria that have 50% smaller (compared to wild-type) Bchl antenna size and display increased sunlight conversion efficiency.
- Complete research to engineer photosynthetic bacteria with a 30% expression level of a functional nitrogenase/hydrogenase at elevated nitrogen-carbon ratios (expression level is defined relative to that detected at low N:C ratios).
- 25 Complete research to inactivate competitive uptake of H₂ by hydrogenase.
- 26 For photosynthetic bacterial hydrogen production, achieve 3% efficiency of incident solar light energy to H₂ (E0*E1*E2) from organic acids, and 50% of maximum molar yield of carbon conversion to H₂ (depends on nature of organic substrate).

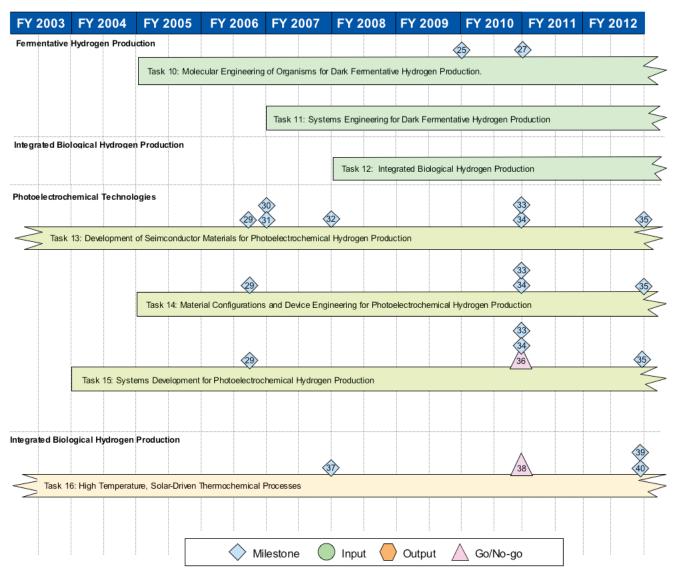
Outputs

- Output to Fuel Cells and Technology Validation: Hydrogen production technology for distributed systems using natural gas with projected cost of \$3.00/gge hydrogen at the pump, untaxed, no carbon sequestration assuming 100s of units of production per year.
- P2 Output to Delivery, Storage and Fuel Cells: Assessment of fuel contaminant composition.
- P3 Output to Systems Analysis and Systems Integration: Impact of hydrogen purity on cost and performance.
- P4 Output to Fuel Cells and Technology Validation: Hydrogen production technology for distributed systems using natural gas with projected cost of \$2.50/gge hydrogen at the pump, untaxed, no carbon sequestration assuming 100s of units of production per year.
- P5 Output to Systems Analysis and Systems Integration: Impact of hydrogen purity on cost and performance.
- P6 Output to Delivery, Storage and Fuel Cells: Assessment of fuel contaminant composition.
- P7 Output to Fuel Cells and Technology Validation: Hydrogen production technologies for distributed systems using natural gas with projected cost of \$1.50/gge hydrogen at the pump, untaxed, no carbon sequestration assuming 100s of units of production per year.
- P8 Output to Technology Validation: Down-select of high-temperature electrolysis technology based on research results.
- P9 Output to Technology Validation: Electrolysis system making hydrogen for \$2.85/gge delivered.
- P10 Output to Technology Validation: Hydrogen production system making hydrogen for \$1.90/gge from biomass at the plant gate.

Inputs

- C3 Input from Codes and Standards: Preliminary Assessment of Safety, Codes and Standards requirements for the hydrogen delivery infrastructure.
- Sf3 Input from Safety: Safety requirements and protocols for refueling.
- C5 Input from Codes and Standards: Completed hydrogen fuel quality standard as ISO Technical Specification.
- A1 Input from Systems Analysis: Complete technoeconomic analysis on production and delivery technologies currently being researched to meet overall Program hydrogen fuel objective.
- F2 Input from Fuel Cells: Research results of advanced reformer development.
- V9 Input from Technology Validation: Final report on safety and O&M of three refueling stations.
- A2 Input from Systems Analysis: Initial recommended hydrogen quality at each point in the system.
- C12 Input from Codes and Standards: Final hydrogen fuel quality standard as ISO Standard.
- Sf5 Input from Safety: Safety requirements and protocols for refueling.

Figure 3.1.3. Hydrogen Production R&D Milestone Chart



For chart details see next page.

Milestones

- 27 For dark fermentative hydrogen production, achieve 4 molar yield of H, production from glucose.
- 28 Complete research to determine the efficacy of green algae/cyanobacteria and photosynthetic bacteria to metabolize carbon substrates (C≤4) and produce H₂ in co-cultivation.
- 29 Update technoeconomic analysis on the projected technology.
- 30 Complete structure and initial data population of a photoelectrochemical materials database.
- 31 Establish standard cell and testing protocols for PEC materials for validation efficiencies.
- 32 Install testing laboratory for the standard cell and testing protocol for PEC materials.
- 33 Update technoeconomic analysis on the projected technology.
- 34 Identify materials/systems with a 2.3 eV useable semiconductor bandgap, 8% plant solar-to-hydrogen efficiency, and projected durability of 1,000 hours.
- 35 Build a consensus, lab-scale PEC panel based on best available 2010 technology to validate technoeconomic analysis.
- 36 Go/No-Go: Identify cost-effective (based on analysis) transparent hydrogen-impermeable material for use in photoelectrochemical hydrogen production system.
- 37 Down-select to 2-4 promising high temperature solar-driven thermochemical cycles for R&D based on analysis and initial laboratory work of potential cycles.
- 38 Go/No-Go: Verify the feasibility of an effective integrated high-temperature solar-driven thermochemical cycle for hydrogen projected to meet the 2010 cost goal of \$4/gge.
- Werify the successful continuous operation of a promising integrated high temperature solar-driven thermochemical cycle at a scale of >10 kg/hr. of hydrogen production.
- 40 Down-select to 1-2 promising high-temperature solar-driven thermochemical cycles for development.

